

Chemistry 125 Second Examination
October 25, 2006

Name _____

The exam budgets 50 minutes, but you may have 60 minutes to finish it. Good answers can fit in the space provided.

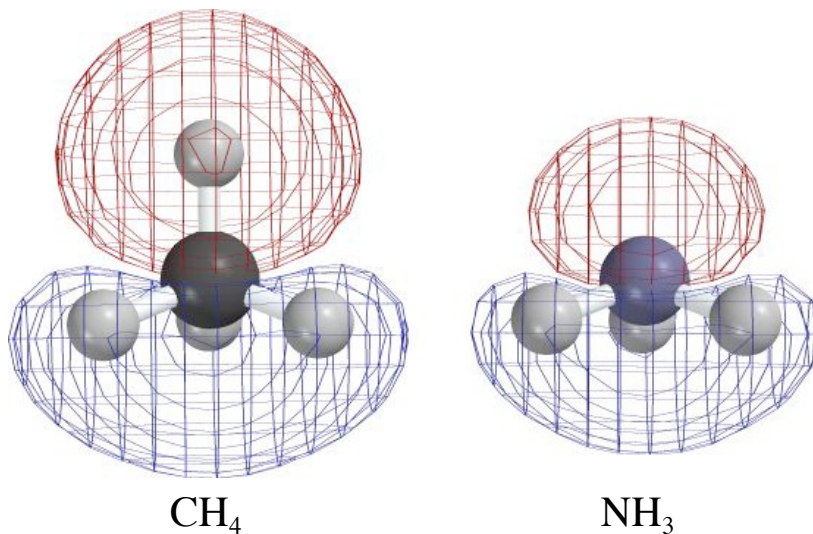
Question values correspond to allotted time. Don't waste too much time on cheap questions.

Read each question carefully to see what it asks for (bold face is used to help highlight questions).

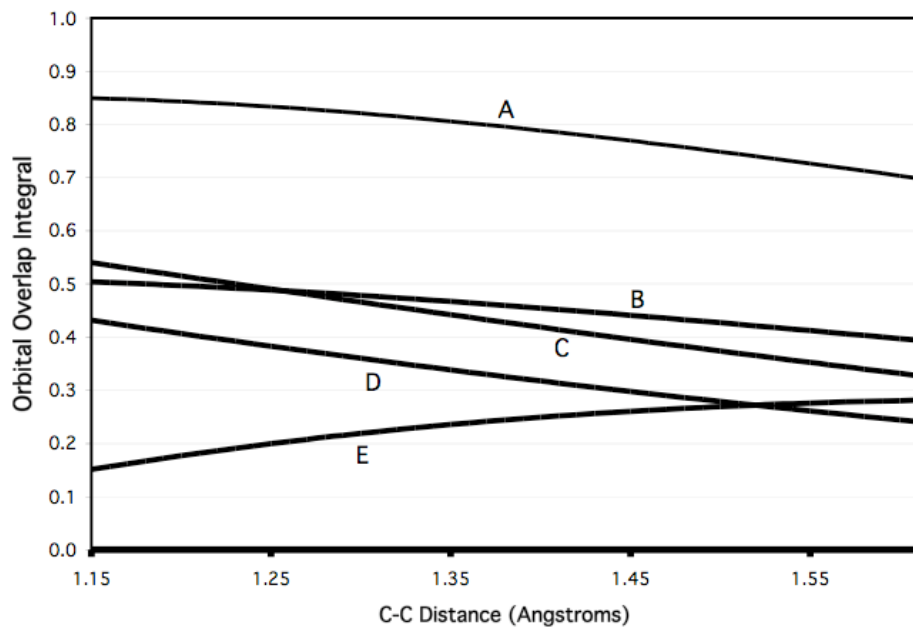
Make sure you are answering the question, not just saying something vaguely relevant to its topic.

1. (1 minute) Altogether about **how long** does it take at the APS source to mount a typical enzyme crystal and collect the x-ray data necessary to determine its molecular structure? _____
2. (4 min) Mention **TWO WAYS** in which the study of Chladni figures in acoustics is relevant to the subject of H-like wave functions.
3. (2 min) Why are H-like wave functions formulated using ρ rather than r to measure distance?
4. (4 min) Explain why solving the quantum mechanical problem of the He atom with three charged particles is MUCH more complicated than solving the H atom with two, **AND NAME** (you need **not** describe) **TWO** methods that are used to address the complication.

5. (4 min) Give **TWO** reasons why it is sensible to formulate a molecular orbital as a weighted sum of atomic orbitals.
6. (4 min) Explain **why**, having formulated an MO as a SUM of atomic orbitals, it is relevant to be interested in a **PRODUCT** of atomic orbitals (the overlap integral). In your answer **mention** both **mathematics** and relevance to **experimental data**.
7. (4 min) CH_4 has the same number of protons and of electrons as does NH_3 . The MOs illustrated for these species have very similar shapes - red lobe above, blue below. **Explain** briefly which of the two orbitals should be higher in energy.



8. (5 min) Give **plausible identifications** for the five pairs of pure or hybrid atomic orbitals of carbon atoms whose overlap integrals at various distances are shown by curves A-E below. In every case but one the two AOs are identical. (Feel free to give brief explanations if you want to be eligible for partial credit despite having made a mistake)



A _____

B _____

C _____

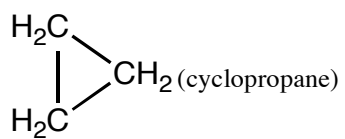
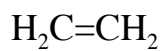
D _____

E _____

9. (3 min) Why are valence orbitals so much more important in making bonds than core orbitals are?

10. (5 min) Why is HOMO/LUMO interaction between two molecules so much more important for reaction than interaction among any other pair of orbitals?

11. (7 min) Explain in terms of orbital energies what makes each of the following 3 molecules reactive:



12. (7 min) **Explain** how **spectroscopic** evidence (**not** x-ray) can be used to show that NH₃ is pyramidal at its minimum of potential energy.